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Degree and Neighborhood Degree Sum-based Topological Characteristics of Zosurabalpin: a Novel Drug for Managing Antibiotic-resistant Infection

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Abstract

This article is concerned with the topological characterization of the antibiotic Zosurabalpin through the computation of degree and associated neighborhood degree sum-based topological indices. The computation of the topological indices is carried out using the mathematical definition as well as with the help of associated graphic polynomials. The geometric representations of the polynomials and numerical values of topological indices are presented graphically. A comparative study between values of degree-based topological indices and associated neighborhood degree sum-based topological indices is

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presented through numerical and graphical representation. The obtained values of topological indices of Zosurabalpin may be helpful to discover the physico-chemical properties of the drug.

Keywords: Zosurabalpin; topological indices; M-polynomial; NM-polynomial.

1 Introduction

The emergence of drug resistant bacteria is a silent pandemic that is undermining the efficacy of fundamental medical treatments and contributing to a rising death toll worldwide. Certain Gram-negative bacteria have gained antibiotic resistance disproportionately. Novel medications against antimicrobial-resistant bacteria, which constitute the biggest threat to human health, are desperately needed [14].

Gram-negative bacteria have a glycolipid covering their surface called lipopolysaccharide (LPS). According to reports, the lipopolysaccharide transport system (Lpt) machinery, a specialized seven-protein transporter system that physically extends across the bacterial cell envelope, is thought to play a significant role in the transport of LPS. LPS is extracted from the inner membrane and transported to the outer membrane by the ABC transporter $LptB_2FG$ complex, which also hydrolyzes ATP. The nucleotide-binding domain component of $LptB_2$ is responsible for binding and hydrolyzing ATP to produce mechanical force for the transportation of LPS. According to reports, the macrocyclic peptide antibiotic Zosurabalpin blocks the transport of LPS by targeting the inner-membrane $LptB_2FGC$ complex. Consequently, this disrupts integration and membrane assembly [26, 29].

Carbapenem-resistant *Acinetobacter baumannii* (CRAB) has become a significant worldwide pathogen as there is no treatment option available for this pathogen. In more than 50 years, no novel antibiotics that are effective against *A. baumannii* have been made available to patients. It has been reported that the above antibiotic Zosurabalpin works well against these pathogens [26, 29]. The two-dimensional chemical structure of Zosurabalpin with hydrogen [28] is depicted in Figure 1.

Before a drug is put on the market, a great deal of study is typically required to determine its tolerability, safety profile, and effectiveness in the human body. Furthermore, these trials necessitate expensive laboratory investigations, state-of-the-art facilities, and substantial financial outlays. In order to comprehend the physico-chemical characteristics, biological

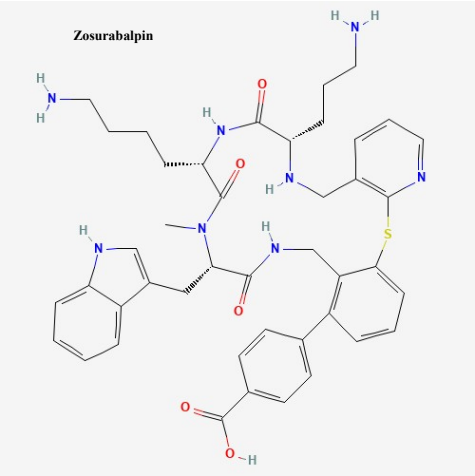


Figure 1: The two-dimensional chemical structures of Zosurabalpin with hydrogen.

activities, and pharmacological behaviours of various chemical compounds, researchers have established impressive connections between their molecular graphs and tests.

Basics of Graph and Topological Indices

Chemical graph theory, which links mathematical chemistry and graph theory, allows for the considerable prediction of certain drug features without the need for any laboratory experiments [6–11, 27]. In this area of graph theory, topological indices provide numerical metrics that represent the molecular characteristics of the molecule. They are particularly used to predict the physico-chemical characteristics and biological activities of the molecular compound through the analysis of *QSPR* (Quantitative Structure-Property Relationship)/*QSAR* (Quantitative Structure-Activity Relationship) models.

Let Υ be a simple, undirected and connected graph represents as an ordered pair $(V(\Upsilon), E(\Upsilon))$, where $V(\Upsilon)$ and $E(\Upsilon)$ denote the vertex set and edge set, respectively. A degree of a vertex s is symbolized by $d_\Upsilon(s)$ and it is defined as $d_\Upsilon(s) = |\{t \in V(\Upsilon) : e = st \in E(\Upsilon)\}|$. The minimum degree and maximum degree of the graph Υ are denoted by δ and Δ, respectively. The neighborhood degree sum of a vertex u is denoted by $\tau_\Upsilon(u)$ and it is described as $\tau_\Upsilon(u) = \{\sum_{v \in V(\Upsilon)} d_\Upsilon(v) : e = uv \in E(\Upsilon)\}$. The minimum

neighborhood degree sum and maximum neighborhood degree sum of the graph Υ are indicated by δ' and Δ', respectively.

As mentioned in [12], the degree-based topological index defined on edge set $E(\Upsilon)$ of a graph Υ can be denoted as

$$TI(\Upsilon) = \sum_{st \in E(\Upsilon)} f(d_\Upsilon(s), d_\Upsilon(t)),$$

where $f(x, y)$ is a non-negative and symmetric function that depends on the mathematical formulation of the topological index. The above definition of the topological index can also be formulated as

$$TI(\Upsilon) = \sum_{\delta \leq p \leq q \leq \Delta} m_{p,q}\ f(p, q),$$

where $m_{p,q}$ is the total number of edges $st \in E(\Upsilon)$ such that $d_\Upsilon(s) = i$, $d_\Upsilon(t) = j$ $(i, j \geq 1)$. The value or expression of the degree-based topological indices can be evaluated using the standard mathematical definition described in Table 1. However, it is a complex approach. In 2015, Deutsch and Klažar introduced the concept of M-polynomial [13] of a graph to compute the degree-based topological indices. Definition of the M-polynomial is described below.

Definition 1 ([13]) *The M-polynomial of a graph Υ defined as*

$$M(\Upsilon; x, y) = \sum_{\delta \leq p \leq q \leq \Delta} m_{p,q}\ x^p y^q,$$

where $\delta = \min\{d_\Upsilon(s) | s \in V(\Upsilon)\}$, $\Delta = \max\{d_\Upsilon(s) | s \in V(\Upsilon)\}$ and $m_{p,q}(\Upsilon)$ is the number of edges $st \in E(\Upsilon)$ such that $d_\Upsilon(s) = p$, $d_\Upsilon(t) = q$ $(p, q \geq 1)$.

The neighborhood degree sum-based topological indices defined on edge set $E(\Upsilon)$ of a graph Υ is denoted as $ND(\Upsilon)$ and mathematically describe as

$$ND(\Upsilon) = \sum_{st \in E(\Upsilon)} f(\tau_\Upsilon(u), \tau_\Upsilon(v)),$$

where $f(\tau_\Upsilon(u), \tau_\Upsilon(v))$ is the function of $\tau_\Upsilon(u)$, $\tau_\Upsilon(v)$ depending on the formal definition of the neighborhood degree sum-based topological indices. As stated in [22], the above definition can also be expressed as

$$ND(\Upsilon) = \sum_{\delta' \leq p \leq q \leq \Delta'} \xi_{p,q} f(p, q).$$

Definition 2 ([24]) *The NM-polynomial of a graph Υ is describe as*

$$NM(\Upsilon; x, y) = \sum_{\delta' \leq p \leq q \leq \Delta'} \xi_{p,q}\ x^p y^q,$$

where $\xi_{p,q}$ $(p, q \geq 1)$ is the number of edges $st \in E(\Upsilon)$ such that $\{\tau_\Upsilon(s), \tau_\Upsilon(t)\} = \{p, q\}$.

The role of the NM-polynomial in determining the neighborhood degree sum-based topological indices is analogous to the M-polynomial in determining the degree-based topological indices. The mathematical definitions of the considered degree-based and neighborhood degree sum-based topological indices are cataloged in Table 1 along with their associated M-polynomial and NM-polynomial-based derivation formulas.

In the article [11], Das et al. applied degree-based topological indices and the M-polynomial approach to the molecular graph of Molnupiravir (a COVID-19 oral antiviral drug) to provide structural and pharmacokinetic insights that may aid the rational design and evaluation of COVID-19 drugs. Further, Das et al. [10] conducted a comprehensive correlation analysis between topological indices and the physico-chemical properties of several COVID-19 antiviral drugs and further established robust *QSPR* models using linear, quadratic and cubic regressions to rigorously evaluate the predictive strength of these indices. Mondal et al. proposed some new indices based on the neighborhood degree sum of vertices and evaluated their predictive capability through *QSPR* regression analysis for the physico-chemical properties of octane isomers and alkanes in the article [23]. In the study [1], Barman and Das computed and analyzed the hyperbolic Sombor index of 22 benzenoid hydrocarbons using curvilinear regression models to evaluate its predictive relationship with key physico-chemical properties. For more literature regarding *QSPR* analysis, interested readers may go through the articles [2–6, 8, 15–21].

Motivation and Methodology

Very recently, the researchers discovered that Zosurabalpin surpassed currently available antibiotics in slowing the growth of difficult-to-treat bacteria and effectively combating CRAB infections in a range of mouse models. Unlike other antibiotics like penicillin, which are naturally occurring byproducts of bacteria or fungus, Zosurabalpin is an artificial substance. In this article, we aim to investigate the topological characterization of the novel

Table 1: Derivation formulas to compute the degree-based and neighbourhood degree sum-based topological indices using the M-polynomial and NM-polynomial of a graph Υ, respectively [10].

Sl. No.	Topological Index	Notation	Formula of topological indices	$f(x,y)$	Derivation from $g(x,y)=M(\Upsilon;x,y)$ or $NM(\Upsilon;x,y)$
1.	First Zagreb Index	$M_1(\Upsilon)$	$\sum_{st\in E(\Upsilon)}(\psi_\Upsilon(s)+\psi_\Upsilon(t))$	$x+y$	$(D_x+D_y)(g(x,y))\|_{x=y=1}$
	Neighborhood First Zagreb Index	$NM_1(\Upsilon)$			
2.	Second Zagreb Index	$M_2(\Upsilon)$	$\sum_{st\in E(\Upsilon)}(\psi_\Upsilon(s)\psi_\Upsilon(t))$	xy	$(D_xD_y)(g(x,y))\|_{x=y=1}$
	Neighborhood Second Zagreb Index	$NM_2(\Upsilon)$			
3.	Modified Second Zagreb Index	${}^mM_2(\Upsilon)$	$\sum_{st\in E(\Upsilon)}\frac{1}{\psi_\Upsilon(s)\psi_\Upsilon(t)}$	$\frac{1}{xy}$	$(S_xS_y)(g(x,y))\|_{x=y=1}$
	Neighborhood Modified Second Zagreb Index	${}^{nm}M_2(\Upsilon)$			
4.	Redefined Third Zagreb Index	$ReZG_3(\Upsilon)$	$\sum_{st\in E(\Upsilon)}(\psi_\Upsilon(s)\psi_\Upsilon(t))(\psi_\Upsilon(s)+\psi_\Upsilon(t))$	$xy(x+y)$	$D_xD_y(D_x+D_y)(g(x,y))\|_{x=y=1}$
	Third NDe Index	$ND_3(\Upsilon)$			
5.	Forgotten Index	$F(\Upsilon)$	$\sum_{st\in E(\Upsilon)}(\psi_\Upsilon(s))^2+(\psi_\Upsilon(t))^2$	x^2+y^2	$(D_x^2+D_y^2)(g(x,y))\|_{x=y=1}$
	Neighborhood Forgotten Index	$NF(\Upsilon)$			
6.	General Randić Index	$R_\alpha(\Upsilon)$	$\sum_{st\in E(\Upsilon)}(\psi_\Upsilon(s)\psi_\Upsilon(t))^\alpha$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(g(x,y))\|_{x=y=1}$
	Neighborhood General Randić Index	$NR_\alpha(\Upsilon)$			
7.	General Inverse Randić Index	$RR_\alpha(\Upsilon)$	$\sum_{st\in E(\Upsilon)}\frac{1}{(\psi_\Upsilon(s)\psi_\Upsilon(t))^\alpha}$	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)(g(x,y))\|_{x=y=1}$
	Neighborhood General Inverse Randić Index	$NRR_\alpha(\Upsilon)$			
8.	Symmetric Division (Deg) Index	$SDD(\Upsilon)$	$\sum_{st\in E(\Upsilon)}\frac{\psi_\Upsilon(s)^2+\psi_\Upsilon(t)^2}{\psi_\Upsilon(s)\psi_\Upsilon(t)}$	$\frac{x^2+y^2}{xy}$	$(D_xS_y+D_yS_x)(g(x,y))\|_{x=y=1}$
	Fifth NDe Index	$ND_5(\Upsilon)$			
9.	Harmonic Index	$H(\Upsilon)$	$\sum_{st\in E(\Upsilon)}\frac{2}{\psi_\Upsilon(s)+\psi_\Upsilon(t)}$	$\frac{2}{x+y}$	$2S_xJ(g(x,y))\|_{x=1}$
	Neighborhood Harmonic Index	$NH(\Upsilon)$			
10.	Inverse Sum (Indeg) Index	$ISI(\Upsilon)$	$\sum_{st\in E(\Upsilon)}\frac{\psi_\Upsilon(s)\psi_\Upsilon(t)}{\psi_\Upsilon(s)+\psi_\Upsilon(t)}$	$\frac{xy}{x+y}$	$S_xJD_xD_y(g(x,y))\|_{x=1}$
	Neighborhood Inverse Sum Index	$NI(\Upsilon)$			
11.	Augmented Zagreb Index	$A(\Upsilon)$	$\sum_{st\in E(\Upsilon)}\left\{\frac{\psi_\Upsilon(s)\psi_\Upsilon(t)}{\psi_\Upsilon(s)+\psi_\Upsilon(t)-2}\right\}^3$	$(\frac{xy}{x+y-2})^3$	$S_x^3Q_{-2}JD_x^3D_y^3(g(x,y))\|_{x=1}$
	Sanskruti Index	$S(\Upsilon)$			

where, $D_x(f(x,y))=x\frac{\partial(f(x,y))}{\partial x}$, $D_y(f(x,y))=y\frac{\partial(f(x,y))}{\partial y}$, $S_x(f(x,y))=\int_0^x\frac{f(t,y)}{t}dt$, $S_y(f(x,y))=\int_0^y\frac{f(x,t)}{t}dt$,
$J(f(x,y))=f(x,x)$, $Q_\alpha(f(x,y))=x^\alpha f(x,y)$, $\alpha\neq 0$,
For degree-based topological indices $\psi_\Upsilon(s)=d_\Upsilon(s)$, $\psi_\Upsilon(t)=d_\Upsilon(t)$ and $g(x,y)=M(\Upsilon;x,y)$.
For neighborhood degree sum-based topological indices $\psi_\Upsilon(s)=\tau_\Upsilon(s)$, $\psi_\Upsilon(t)=\tau_\Upsilon(t)$ and $g(x,y)=NM(\Upsilon;x,y)$.
For $\alpha=-1/2$, $NRR_\alpha(\Upsilon)$ is known as first NDe index and it is denoted by ND_1.

antibiotic drug Zosurabalpin through the computation of the degree-based and neighborhood degree sum-based topological indices. At the outset in Section 2, we demonstrate the hydrogen-surpassed 2D molecular graph with degree of each vertex of Zosurabalpin and compute the vertex set and edge set partitions. The computation of degree-based topological indices

of Zosurabalpin is carried out using their mathematical definitions and M-polynomial-based derivation formula approach. The geometrical behavior of the M-polynomial and degree-based topological indices of Zosurabalpin are also shown graphically. In Section 3, the neighborhood degree sum-based topological indices are calculated using their standard mathematical definitions as well as NM-polynomial method. Further, we demonstrate the geometrical behavior of the NM-polynomial and plot the neighborhood degree sum-based topological indices in increasing order. Section 4 presents the comparative study between the degree and neighborhood degree-based topological indices through numerical and graphical approaches. MATLAB R2019a software is used for the geometrical plots of graphic polynomials, whereas MS Excel is used for plotting the values of topological indices. Section 5 is reserved for concluding the remarks.

2 Degree-Based Topological Indices of Zosurabalpin

In the computation of topological index, hydrogen atoms are usually ignored, because the hydrogen atoms (vertices) do not affect the graph isomorphism [25]. In Figure 2, we depict the hydrogen-supressed molecular graph of Zosurabalpin, which we denote using the notation Υ throughout this article. Moreover, the degree of each vertex is shown in this figure itself. Let us first compute some significant graph invariants and properties of the graph Υ before moving to the further investigation:

1. Total number of elements in vertex set $V(\Upsilon)$ and edge set $E(\Upsilon)$ of Υ are:
$$|V(\Upsilon)| = 57 \quad \text{and} \quad |E(\Upsilon)| = 62.$$

2. The graph Υ have vertices of degree $1, 2$ and 3, i.e. $d_\Upsilon(s)$ is either 1 or 2 or 3 for every $s \in V(\Upsilon)$.

3. As per the possible degree of vertices, the vertex set $V(\Upsilon)$ can be partition in three disjoint sets. The partitions set are as follows:
$$V_p(\Upsilon) = \{s \in V(\Upsilon) : d_\Upsilon(s) = p, \text{ where } p = 1, 2 \text{ and } 3\},$$
the total number of vertices in all the three partitions of the vertex set is given as:
$$|V_1(\Upsilon)| = 8, \ |V_2(\Upsilon)| = 31 \ \text{ and } \ |V_3(\Upsilon)| = 18.$$

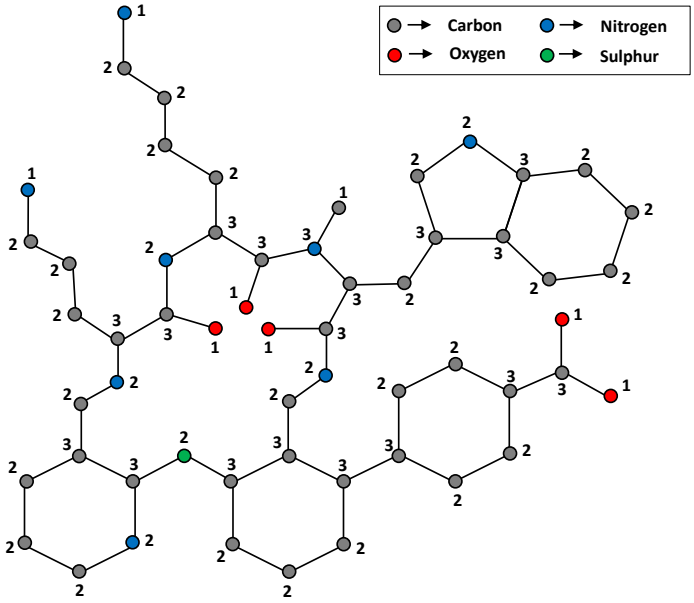


Figure 2: The hydrogen-suppressed molecular graph of Zosurabalpin with degree of each vertex.

4. According to the degrees of end vertices of an edge $e = st \in E(\Upsilon)$, the partitions of the edge set $E(\Upsilon)$ are as follows:

$$E_{\{p,q\}} = \{e = st \in E(\Upsilon) : d_\Upsilon(s) = p, d_\Upsilon(t) = q\},$$

where $\{p, q\} = \{1, 2\}, \{1, 3\}, \{2, 2\}, \{2, 3\}$ and $\{3, 3\}$

and the total number of edges in $E_{\{p,q\}}$ are given as

$|E_{\{1,2\}}| = 2, |E_{\{1,3\}}| = 6, |E_{\{2,2\}}| = 18, |E_{\{2,3\}}| = 24$ and $|E_{\{3,3\}}| = 12$.

Now, we utilize the standard mathematical definitions as cataloged in Table 1 to examine the degree-based topological indices of Zosurabalpin.

Theorem 3 *Let Υ be the hydrogen-surpassed 2D-molecular graph of Zosurabalpin. Then, the degree-based topological indices of Υ are*

(i) $M_1(\Upsilon) = 294$,

(ii) $M_2(\Upsilon) = 346$,

(iii) ${}^{m}M_2(\Upsilon) = \frac{77}{6} \approx 12.8333$,

(iv) $ReZG_3(\Upsilon) = 1,740$,

(v) $F(\Upsilon) = 742$,

(vi) $R_\alpha(\Upsilon) = 2^{\alpha+1} + 2 \times 3^{\alpha+1} + 9 \times 2^{2\alpha+1} + 4 \times 2^{\alpha+3} \times 3^{\alpha+1} + 4 \times 3^{2\alpha+1}$,

(vii) $RR_\alpha(\Upsilon) = \frac{1}{2^{\alpha-1}} + \frac{2}{3^{\alpha-1}} + \frac{9}{2^{2\alpha-1}} + \frac{4}{6^{\alpha-1}} + \frac{4}{3^{2\alpha-1}}$,

(viii) $SDD(\Upsilon) = 137$,

(ix) $H(\Upsilon) = \frac{404}{15} \approx 26.9333$,

(x) $ISI(\Upsilon) = \frac{2,119}{30} \approx 70.6333$,

(xi) $AZI(\Upsilon) = \frac{8,143}{16} \approx 508.9375$.

Proof: Computation of degree-based topological indices of Zosurabalpin using the standard mathematical definitions as listed in Table 1 is presented below in a following way:

(i) **First Zagreb index:**

$$\begin{aligned} M_1(\Upsilon) &= \sum_{st \in E(\Upsilon)} (d_\Upsilon(s) + d_\Upsilon(t)) \\ &= 2(1+2) + 6(1+3) + 18(2+2) + 24(2+3) + 12(3+3) \\ &= 294. \end{aligned}$$

(ii) **Second Zagreb index:**

$$\begin{aligned} M_2(\Upsilon) &= \sum_{st \in E(\Upsilon)} (d_\Upsilon(s) d_\Upsilon(t)) \\ &= 2(1 \times 2) + 6(1 \times 3) + 18(2 \times 2) + 24(2 \times 3) + 12(3 \times 3) \\ &= 346. \end{aligned}$$

(iii) **Modified second Zagreb index:**

$$\begin{aligned} {}^{m}M_2(\Upsilon) &= \sum_{st \in E(\Upsilon)} \frac{1}{d_\Upsilon(s) d_\Upsilon(t)} \\ &= \frac{2}{1 \times 2} + \frac{6}{1 \times 3} + \frac{18}{2 \times 2} + \frac{24}{2 \times 3} + \frac{12}{3 \times 3} \\ &= \frac{77}{6} \approx 12.8333. \end{aligned}$$

(iv) **Redefined third Zagreb index:**

$$\begin{aligned} ReZG_3(\Upsilon) &= \sum_{st\in E(\Upsilon)} d_\Upsilon(s)d_\Upsilon(t)(d_\Upsilon(s)+d_\Upsilon(t)) \\ &= 2(1\times 2)(1+2)+6(1\times 3)(1+3)+18(2\times 2)(2+2) \\ &\quad +24(2\times 3)(2+3)+12(3\times 3)(3+3) \\ &= 1,740. \end{aligned}$$

(v) **Forgotten index:**

$$\begin{aligned} F(\Upsilon) &= \sum_{st\in E(\Upsilon)} (d_\Upsilon(s)^2+d_\Upsilon(t)^2) \\ &= 2(1+4)+6(1+9)+18(4+4)+24(4+9)+12(9+9) \\ &= 742. \end{aligned}$$

(vi) **General Randić index:**

$$\begin{aligned} R_\alpha(\Upsilon) &= \sum_{st\in E(\Upsilon)} (d_\Upsilon(s)d_\Upsilon(t))^\alpha \\ &= 2(1\times 2)^\alpha+6(1\times 3)^\alpha+18(2\times 2)^\alpha+24(2\times 3)^\alpha+12(3\times 3)^\alpha \\ &= 2^{\alpha+1}+2\times 3^{\alpha+1}+9\times 2^{2\alpha+1}+4\times 2^{\alpha+3}\times 3^{\alpha+1}+4\times 3^{2\alpha+1}. \end{aligned}$$

(vii) **General inverse Randić index:**

$$\begin{aligned} RR_\alpha(\Upsilon) &= \sum_{st\in E(\Upsilon)} \frac{1}{(d_\Upsilon(s)d_\Upsilon(t))^\alpha} \\ &= \frac{2}{(1\times 2)^\alpha}+\frac{6}{(1\times 3)^\alpha}+\frac{18}{(2\times 2)^\alpha}+\frac{24}{(2\times 3)^\alpha}+\frac{12}{(3\times 3)^\alpha} \\ &= \frac{1}{2^{\alpha-1}}+\frac{2}{3^{\alpha-1}}+\frac{9}{2^{2\alpha-1}}+\frac{4}{6^{\alpha-1}}+\frac{4}{3^{2\alpha-1}}. \end{aligned}$$

(viii) **Symmetric division deg index:**

$$\begin{aligned} SDD(\Upsilon) &= \sum_{st\in E(\Upsilon)} \left\{\frac{d_\Upsilon(s)}{d_\Upsilon(t)}+\frac{d_\Upsilon(t)}{d_\Upsilon(s)}\right\} \\ &= 2\left\{\frac{1}{2}+\frac{2}{1}\right\}+6\left\{\frac{1}{3}+\frac{3}{1}\right\}+18\left\{\frac{2}{2}+\frac{2}{2}\right\}+24\left\{\frac{2}{3}+\frac{3}{2}\right\} \end{aligned}$$

$$
\begin{aligned}
&+ 12\left\{\frac{3}{3}+\frac{3}{3}\right\}\\
&= 5 + 20 + 36 + 52 + 21\\
&= 137.
\end{aligned}
$$

(ix) **Harmonic index:**

$$
\begin{aligned}
H(\Upsilon) &= \sum_{st\in E(\Upsilon)} \frac{2}{d_\Upsilon(s)+d_\Upsilon(t)}\\
&= 2\left\{\frac{2}{1+2}\right\} + 6\left\{\frac{2}{1+3}\right\} + 18\left\{\frac{2}{2+2}\right\} + 24\left\{\frac{2}{2+3}\right\}\\
&\quad + 18\left\{\frac{2}{3+3}\right\}\\
&= \frac{404}{15} \approx 26.9333.
\end{aligned}
$$

(x) **Inverse sum indeg index:**

$$
\begin{aligned}
ISI(\Upsilon) &= \sum_{st\in E(\Upsilon)} \frac{d_\Upsilon(s)d_\Upsilon(t)}{d_\Upsilon(s)+d_\Upsilon(t)}\\
&= 2\left\{\frac{1\times 2}{1+2}\right\} + 6\left\{\frac{1\times 3}{1+3}\right\} + 18\left\{\frac{2\times 2}{2+2}\right\} + 24\left\{\frac{2\times 3}{2+3}\right\}\\
&\quad + 12\left\{\frac{3\times 3}{3+3}\right\}\\
&= \frac{2,119}{30} \approx 70.6333.
\end{aligned}
$$

(xi) **Augmented Zagreb index:**

$$
\begin{aligned}
AZI(\Upsilon) &= \sum_{st\in E(\Upsilon)} \left\{\frac{d_\Upsilon(s)d_\Upsilon(t)}{d_\Upsilon(s)+d_\Upsilon(t)-2}\right\}^3\\
&= 2\left\{\frac{1\times 2}{1+2-2}\right\}^3 + 6\left\{\frac{1\times 3}{1+3-2}\right\}^3 + 18\left\{\frac{2\times 2}{2+2-2}\right\}^3\\
&\quad + 24\left\{\frac{2\times 3}{2+3-2}\right\}^3 + 12\left\{\frac{3\times 3}{3+3-2}\right\}^3\\
&= \frac{8,143}{16} \approx 508.9375.
\end{aligned}
$$

□

Next, we discover the closed algebraic expression of the M-polynomial of Zosurabalpin in Theorem 4 using edge partition method and computational techniques.

Theorem 4 *Let Υ be the molecular graph of Zosurabalpin. Then the expression of M-polynomial of Υ is given as*

$$M(\Upsilon; x, y) = 2x^1y^2 + 6x^1y^3 + 18x^2y^2 + 24x^2y^3 + 12x^3y^3.$$

Proof: Here, Υ be the molecular graph of Zosurabalpin as shown in Figure 2. The graph Υ has total 57 vertices and 62 edges, i.e. $|V(\Upsilon)| = 57$ and $|E(\Upsilon)| = 62$. Further, as discussed earlier, the edge set of the graph Υ has total five partition sets as per the degrees of end vertices of an edge. The five partition sets are as follows:

$$E_{\{p,q\}} = \{e = st \in E(\Upsilon) : d_\Upsilon(s) = p, d_\Upsilon(t) = q\},$$

where $\{p, q\} = \{1, 2\}, \{1, 3\}, \{2, 2\}, \{2, 3\}$ and $\{3, 3\}$. Their cardinalities are given as $|E_{\{1,2\}}| = 2$, $|E_{\{1,3\}}| = 6, |E_{\{2,2\}}| = 18, |E_{\{2,3\}}| = 24$ and $|E_{\{3,3\}}| = 12$. Therefore, by using Definition 1, we obtain the closed algebraic expression of the M-polynomial of the graph Υ as follows:

$$\begin{aligned}
M(\Upsilon; x, y) &= \sum_{\delta \le p \le q \le \Delta} m_{p,q}\, x^p y^q, \quad \text{where} \quad p, q \in \{1, 2, 3\} \\
&= \sum_{1 \le 2} m_{1,2}\, x^1y^2 + \sum_{1 \le 3} m_{1,3}\, x^1y^3 + \sum_{2 \le 2} m_{2,2}\, x^2y^2 + \sum_{2 \le 3} m_{2,3}\, x^2y^3 \\
&\quad + \sum_{3 \le 3} m_{3,3}\, x^3y^3 \\
&= \sum_{e=uv \in E_{\{1,2\}}} m_{1,2}\, x^1y^2 + \sum_{e=uv \in E_{\{1,3\}}} m_{1,3}\, x^1y^3 + \sum_{uv \in E_{\{2,2\}}} m_{2,2}\, x^2y^2 \\
&\quad + \sum_{e=uv \in E_{\{2,3\}}} m_{2,3}\, x^2y^3 + \sum_{e=uv \in E_{\{3,3\}}} m_{3,3}\, x^3y^3 \\
&= |E_{\{1,2\}}|\, x^1y^2 + |E_{\{1,3\}}|\, x^1y^3 + |E_{\{2,2\}}|\, x^2y^2 + |E_{\{2,3\}}|\, x^2y^3 \\
&\quad + |E_{\{3,3\}}|\, x^3y^3 \\
&= 2x^1y^2 + 6x^1y^3 + 18x^2y^2 + 24x^2y^3 + 12x^3y^3.
\end{aligned}$$

□

In addition, we present the alternative proof of Theorem 3 to extract the different considered degree-based topological indices of graph Υ using the M-polynomial expression proved in Theorem 4 and derivation formulas listed in Table 1.

Proof: (*Alternative proof of Theorem* 3 via M-polynomial approach). To avoid the notation complexity, let us first denote $g(x,y) = M(\Upsilon; x, y)$. Therefore, the M-polynomial for the graph Υ (as proved in Theorem 4) is

$$g(x,y) = 2x^1y^2 + 6x^1y^3 + 18x^2y^2 + 24x^2y^3 + 12x^3y^3.$$

Next, the computation of some essential operators and their combination is given as follows:

- $D_x(g(x,y)) = 2x^1y^2 + 6x^1y^3 + 36x^2y^2 + 48x^2y^3 + 36x^3y^3$,
- $D_y(g(x,y)) = 4x^1y^2 + 18x^1y^3 + 36x^2y^2 + 72x^2y^3 + 36x^3y^3$,
- $D_xD_y(g(x,y)) = 4x^1y^2 + 18x^1y^3 + 72x^2y^2 + 144x^2y^3 + 108x^3y^3$,
- $(D_x + D_y)(g(x,y)) = 6x^1y^2 + 24x^1y^3 + 72x^2y^2 + 120x^2y^3 + 72x^3y^3$,
- $D_xD_y(D_x + D_y)(g(x,y)) = 12x^1y^2 + 72x^1y^3 + 288x^2y^2 + 720x^2y^3 + 648x^3y^3$,
- $S_x(g(x,y)) = 2x^1y^2 + 6x^1y^3 + 9x^2y^2 + 12x^2y^3 + 4x^3y^3$,
- $D_yS_x(g(x,y)) = 4x^1y^2 + 18x^1y^3 + 18x^2y^2 + 36x^2y^3 + 12x^3y^3$,
- $S_y(g(x,y)) = x^1y^2 + 2x^1y^3 + 9x^2y^2 + 8x^2y^3 + 4x^3y^3$,
- $D_xS_y(g(x,y)) = x^1y^2 + 2x^1y^3 + 18x^2y^2 + 16x^2y^3 + 12x^3y^3$,
- $S_xS_y(g(x,y)) = x^1y^2 + 2x^1y^3 + \frac{9}{2}x^2y^2 + 4x^2y^3 + \frac{4}{3}x^3y^3$,
- $D_x^{\alpha}D_y^{\alpha}(g(x,y)) = 2^{\alpha+1}x^1y^2 + 2 \times 3^{\alpha+1}x^1y^3 + 9 \times 2^{2\alpha+1}x^2y^2 + 4 \times 6^{\alpha+1}x^2y^3 + 4 \times 3^{2\alpha+1}x^3y^3$,
- $S_x^{\alpha}S_y^{\alpha}(g(x,y)) = \frac{1}{2^{\alpha-1}}x^1y^2 + \frac{2}{3^{\alpha-1}}x^1y^3 + \frac{9}{2^{2\alpha-1}}x^2y^2 + \frac{4}{6^{\alpha-1}}x^2y^3 + \frac{4}{3^{2\alpha-1}}x^3y^3$,
- $(D_xS_y + D_yS_x)(g(x,y)) = 5x^1y^2 + 20x^1y^3 + 36x^2y^2 + 52x^2y^3 + 24x^3y^3$,
- $S_xJ(g(x,y)) = \frac{2}{3}x^3 + 6x^4 + \frac{24}{5}x^5 + 2x^6$,
- $S_xJD_xD_y(g(x,y)) = \frac{4}{3}x^3 + \frac{45}{2}x^4 + \frac{144}{5}x^5 + 18x^6$,

- $S_x^3 Q_{-2} J D_x^3 D_y^3(g(x,y)) = 16x + \frac{657}{4}x^2 + 192x^3 + \frac{2{,}187}{16}x^4$.

Thus, employing the M-polynomial-based derivation formulas given in Table 1, we obtain the degree-based topological indices of the Υ as follows:

(i) **First Zagreb index:**

$$M_1(\Upsilon) = (D_x + D_y)(g(x,y))|_{x=y=1} = 294.$$

(ii) **Second Zagreb index:**

$$M_2(\Upsilon) = D_x D_y(g(x,y))|_{x=y=1} = 346.$$

(iii) **Modified second Zagreb index:**

$${}^{m}M_2(\Upsilon) = S_x S_y(g(x,y))|_{x=y=1} = \frac{31}{6} \approx 12.8333.$$

(iv) **Redefined third Zagreb index:**

$$ReZG_3(\Upsilon) = D_x D_y(D_x + D_y)(g(x,y))|_{x=y=1} = 1,740.$$

(v) **Forgotten index:**

$$F(\Upsilon) = (D_x^2 + D_y^2)(g(x,y))|_{x=y=1} = 742.$$

(vi) **General Randić index:**

$$\begin{aligned} R_\alpha(\Upsilon) &= D_x^\alpha D_y^\alpha(g(x,y))|_{x=y=1} \\ &= 2^{\alpha+1} + 2 \times 3^{\alpha+1} + 9 \times 2^{2\alpha+1} + 4 \times 2^{\alpha+3} \times 3^{\alpha+1} + 4 \times 3^{2\alpha+1}. \end{aligned}$$

(vii) **General inverse Randić index:**

$$\begin{aligned} RR_\alpha(\Upsilon) &= S_x^\alpha S_y^\alpha(g(x,y))|_{x=y=1} \\ &= \frac{1}{2^{\alpha-1}} + \frac{2}{3^{\alpha-1}} + \frac{9}{2^{2\alpha-1}} + \frac{4}{6^{\alpha-1}} + \frac{4}{3^{2\alpha-1}}. \end{aligned}$$

(viii) **Symmetric division deg index:**

$$SDD(\Upsilon) = (D_x S_y + D_y S_x)(g(x,y))|_{x=y=1} = 137.$$

(ix) **Harmonic index:**

$$H(\Upsilon) = 2S_xJ(g(x,y))|_{x=1} = \frac{404}{15} \approx 26.9333.$$

(x) **Inverse Sum indeg index:**

$$ISI(\Upsilon) = S_xJD_xD_y(g(x,y))|_{x=1} = \frac{2,119}{30} \approx 70.6333.$$

(xi) **Augmented Zagreb index:**

$$AZI(\Upsilon) = S_x^3Q_{-2}JD_x^3D_y^3(g(x,y))|_{x=1} = \frac{8,143}{16} \approx 508.9375.$$

□

Corollary 5 *Theorem 3 shows that the expression of the general Randić index of a graph Υ is given as $R_\alpha(\Upsilon) = 2^{\alpha+1} + 2 \times 3^{\alpha+1} + 9 \times 2^{2\alpha+1} + 4 \times 2^{\alpha+3} \times 3^{\alpha+1} + 4 \times 3^{2\alpha+1}$. For $\alpha = -1/2$, It is known as the Randić index of Υ and its value is $R_{-1/2}(\Upsilon) = 27.6763$.*

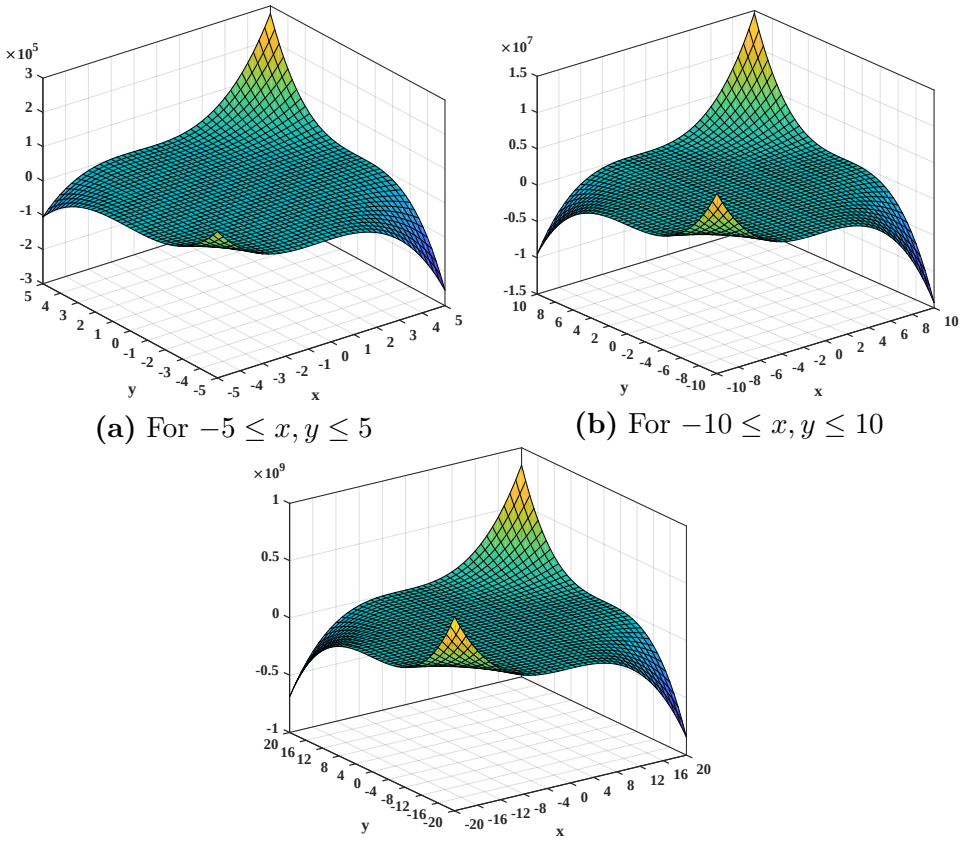
Corollary 6 *On the the hand, Theorem 3 demonstrates that the expression of the general inverse Randić index of a graph Υ is obtained by $RR_\alpha(\Upsilon) = \frac{1}{2^{\alpha-1}} + \frac{2}{3^{\alpha-1}} + \frac{9}{2^{2\alpha-1}} + \frac{4}{6^{\alpha-1}} + \frac{4}{3^{2\alpha-1}}$. For $\alpha = -1/2$, $RR_\alpha(\Upsilon)$ is known as the inverse Randić index of Υ and its value is given by $RR_{-1/2}(\Upsilon) = 144.0085$.*

Remark 7 *The obtained numerical values of the considered different degree-based topological indices from M-polynomial method are equal to their acquired values calculated by using the standard mathematical definitions.*

Additionally, we plot the 3D-surface plot of the M-polynomial and numerical values of associated degree-based topological indices of the Zosurabalpin graphically. The surface representation of the M-polynomial is presented in Figure 3 for different ranges of x and y using MATLAB R2019a software. For instance, Figure 3(a) for $-5 \leq x, y \leq 5$, Figure 3(b) for $-10 \leq x, y \leq 10$ and Figure 3(c) for $-20 \leq x, y \leq 20$ show the geometrical behaviour of the M-polynomial in different regions. Although these surfaces appear to exhibit similar behaviours, their gradients vary differently in different regions. Keep in mind that we may control the M-polynomial value using the parameters x and y. Further, the numerical values of the considered degree-based topological indices are plotted in their increasing

order using MS Excel software on a graph, as shown in Figure 4. From Figure 4, one can observe that the redefined third Zagreb index ($ReZG_3$) reports the highest value $1,740$, while the modified second Zagreb index (${}^mM_2$) has the lowest value 12.8333. All the considered topological indices maintain the following inequality relationship:

$${}^mM_2 < H < R_{-1/2} < ISI < SDD < RR_{-1/2} < M_1 < M_2 < AZI < F < ReZG_3.$$



(a) For $-5 \leq x, y \leq 5$

(b) For $-10 \leq x, y \leq 10$

(c) For $-20 \leq x, y \leq 20$

Figure 3: Surface depiction of M-polynomial of Zosurabalpin for different regions of x and y.

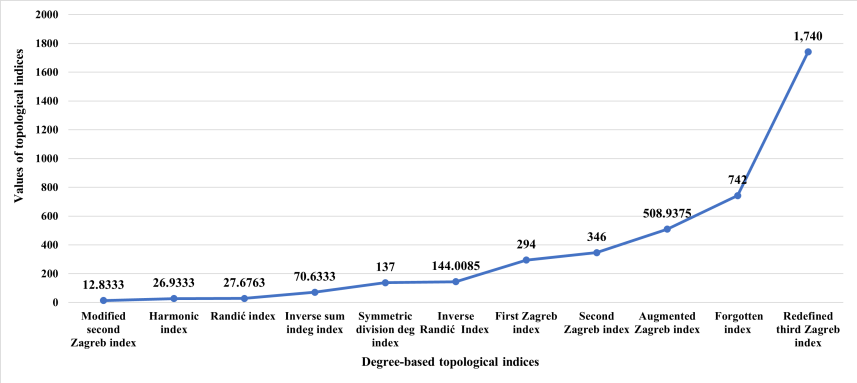


Figure 4: Graphical plot of the numerical values of degree-based topological indices of Zosurabalpin in increasing order.

3 Neighborhood Degree Sum-based Topological Indices of Zosurabalpin

This segment commenced with the computation of some significant graph invariant and properties of the molecular graph Υ represented in Figure 5 of the Zosurabalpin. The associated graph invariant and properties of the graph Υ are as follows:

1. The total counts of elements in the vertex and edge sets of the graph Υ are 57 and 62, respectively.

2. The only possible neighborhood degree-sum of the vertices are 2, 3, 4, 5, 6, 7 and 8, i.e. $\tau_\Upsilon(s) = 2 - 8$ for every $s \in V(\Upsilon)$.

3. According to the neighborhood degree-sum of a vertex, the vertex set $V(\Upsilon)$ have the eight distinct partitions set. The sets and their cardinalities are as follows:

$$V_p^*(\Upsilon) = \{s \in V(\Upsilon) | \tau_\Upsilon(s) = p \text{ where } p = 2,\ 3,\ 4,\ 5,\ 6,\ 7 \text{ and } 8\},$$

and $|V_2^*| = 2$, $|V_3^*| = 8$, $|V_4^*| = 8$, $|V_5^*| = 19$, $|V_6^*| = 5$, $|V_7^*| = 11$ and $|V_8^*| = 4$.

4. The edge set partitions according to the neighborhood degree-sum of end vertices of an edge are described as:

$$E_{\{p,q\}}^* = \{e = st \in E(\Upsilon) : \tau_\Upsilon(s) = p, \tau_\Upsilon(t) = q\},$$

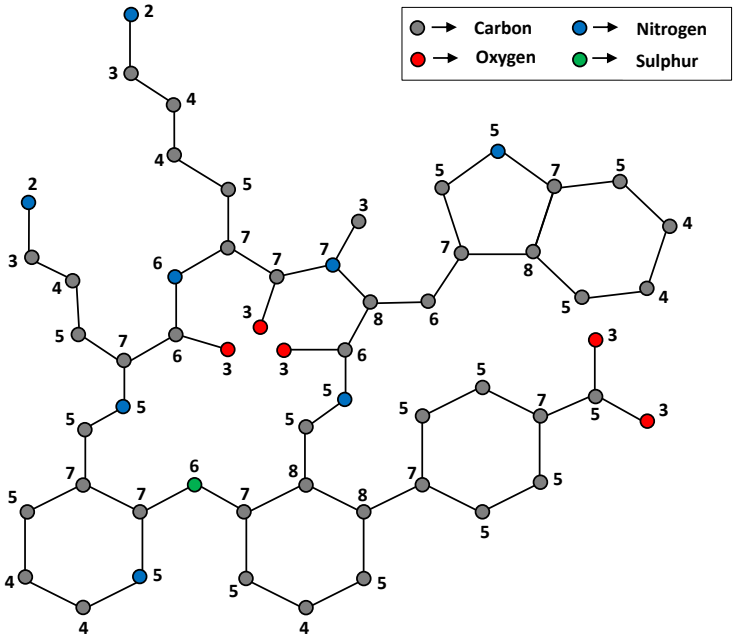


Figure 5: The hydrogen-suppressed 2D-molecular graph of Zosurabalpin with the neighborhood degree-sum of each vertex.

where $\{p,q\} = \{2,3\}$, $\{3,4\}$, $\{3,5\}$, $\{3,6\}$, $\{3,7\}$, $\{4,4\}$, $\{4,5\}$,$\{5,5\}$, $\{5,6\}$, $\{5,7\}$, $\{5,8\}$,$\{6,6\}$, $\{6,7\}$,, $\{6,8\}$, $\{7,7\}$ $\{7,8\}$ and $\{8,8\}$, and the cardinalities of the edge partition sets are given by $|E^*_{\{2,3\}}| = 2$, $|E^*_{\{3,4\}}| = 2$, $|E^*_{\{3,5\}}| = 2$, $|E^*_{\{3,6\}}| = 2$, $|E^*_{\{3,7\}}| = 2$, $|E^*_{\{4,4\}}| = 3$, $|E^*_{\{4,5\}}| = 8$, $|E^*_{\{5,5\}}| = 5$, $|E^*_{\{5,6\}}| = 1$, $|E^*_{\{5,7\}}| = 15$, $|E^*_{\{5,8\}}| = 3$, $|E^*_{\{6,6\}}| = 1$, $|E^*_{\{6,7\}}| = 5$, $|E^*_{\{6,8\}}| = 2$, $|E^*_{\{7,7\}}| = 3$, $|E^*_{\{7,8\}}| = 5$ and $|E^*_{\{8,8\}}| = 1$.

Next, the computational approach is presented to compute the considered different neighborhood degree-sum-based topological indices using their standard mathematical definitions.

Theorem 8 *Let Υ represents the molecular graph of Zosurabalpin shown in Figure 5. Then, the neighborhood degree-based topological indices of Υ are*

(i) $NM_1(\Upsilon) = 692$,

(ii) $NM_2(\Upsilon) = 1985$,

(iii) ${}^{nm}M_2(\Upsilon) = \frac{355441}{141120} \approx 2.5187$,

(iv) $ND_3(\Upsilon) = 24264$,

(v) $NF(\Upsilon) = 4146$,

(vi) $NR_\alpha(\Upsilon) = 2^{\alpha+1} \times 3^\alpha + 2^{2\alpha+1} \times 3^\alpha + 2 \times 15^\alpha + 2^{\alpha+1} \times 3^{2\alpha} + 2 \times 21^\alpha + 3 \times 2^{4\alpha} + 2^{2\alpha+3} \times 5^\alpha + 5^{2\alpha+1} + 30^\alpha + 3 \times 5^{\alpha+1} \times 7^\alpha + 3 \times 2^{3\alpha} \times 5^\alpha + 6^{2\alpha} + 5 \times 42^\alpha + 2^{4\alpha+1} \times 3^\alpha + 3 \times 7^{2\alpha} + 5 \times 2^{3\alpha} \times 7^\alpha + 2^{6\alpha}$,

(vii) $NRR_\alpha(\Upsilon) = \frac{1}{2^{\alpha-1}\times 3^\alpha} + \frac{2}{3^\alpha \times 4^\alpha} + \frac{2}{3^\alpha \times 5^\alpha} + \frac{2}{3^\alpha \times 6^\alpha} + \frac{2}{3^\alpha \times 7^\alpha} + \frac{3}{4^{2\alpha}} + \frac{8}{4^\alpha \times 5^\alpha} + \frac{1}{5^{2\alpha-1}} + \frac{1}{5^\alpha \times 6^\alpha} + \frac{15}{5^\alpha \times 7^\alpha} + \frac{3}{5^\alpha \times 8^\alpha} + \frac{1}{6^{2\alpha}} + \frac{5}{6^\alpha \times 7^\alpha} + \frac{2}{6^\alpha \times 8^\alpha} + \frac{3}{7^{2\alpha}} + \frac{5}{7^\alpha \times 8^\alpha} + \frac{1}{8^{2\alpha}}$,

(viii) $ND_5(\Upsilon) = \frac{54917}{420} \approx 130.7548$,

(ix) $NH(\Upsilon) = \frac{4262647}{360360} \approx 11.8289$,

(x) $NI(\Upsilon) = \frac{15219989}{90090} \approx 168.9420$,

(xi) $S(\Upsilon) = \frac{4364153715096106937}{1733189185728000} \approx 2517.9904$.

Proof: The procedure to compute the neighborhood degree sum-based topological indices of the Zosurabalpin using their standard mathematical formulas cataloged in Table 1 is shown in a following manner:

(i) **Neighborhood first Zagreb index:**

$$\begin{aligned} NM_1(\Upsilon) &= \sum_{st \in E(\Upsilon)} (\tau_\Upsilon(s) + \tau_\Upsilon(t)) \\ &= 2(2+3) + 2(3+4) + 2(3+5) + 2(3+6) + 2(3+7) \\ &\quad + 3(4+4) + 8(4+5) + 5(5+5) + (5+6) + 15(5+7) \\ &\quad + 3(5+8) + (6+6) + 5(6+7) + 2(6+8) + 3(7+7) \\ &\quad + 5(7+8) + (8+8) \\ &= 692. \end{aligned}$$

(ii) **Neighborhood second Zagreb index:**

$$\begin{aligned} NM_2(\Upsilon) &= \sum_{st \in E(\Upsilon)} (\tau_\Upsilon(s)\tau_\Upsilon(t)) \\ &= 2(2\times 3) + 2(3\times 4) + 2(3\times 5) + 2(3\times 6) + 2(3\times 7) \\ &\quad + 3(4\times 4) + 8(4\times 5) + 5(5\times 5) + (5\times 6) + 15(5\times 7) \end{aligned}$$

$$
\begin{aligned}
&+ 3(5\times 8) + (6\times 6) + 5(6\times 7) + 2(6\times 8) + 3(7\times 7)\\
&+ 5(7\times 8) + (8\times 8)\\
&= 1985.
\end{aligned}
$$

(iii) **Neighborhood modified second Zagreb index:**

$$
\begin{aligned}
{}^{nm}M_2(\Upsilon) &= \sum_{st\in E(\Upsilon)} \frac{1}{\tau_\Upsilon(s)\tau_\Upsilon(t)}\\
&= \frac{2}{2\times 3} + \frac{2}{3\times 4} + \frac{2}{3\times 5} + \frac{2}{3\times 6} + \frac{2}{3\times 7} + \frac{3}{4\times 4} + \frac{8}{4\times 5}\\
&\quad + \frac{5}{5\times 5} + \frac{1}{5\times 6} + \frac{15}{5\times 7} + \frac{3}{5\times 8} + \frac{1}{6\times 6} + \frac{5}{6\times 7} + \frac{2}{6\times 8}\\
&\quad + \frac{3}{7\times 7} + \frac{5}{7\times 8} + \frac{1}{8\times 8}\\
&= \frac{355441}{141120} \approx 2.5187.
\end{aligned}
$$

(iv) **Third NDe index:**

$$
\begin{aligned}
ND_3(\Upsilon) &= \sum_{st\in E(\Upsilon)} \tau_\Upsilon(s)\tau_\Upsilon(t)(\tau_\Upsilon(s) + \tau_\Upsilon(t))\\
&= 2(2\times 3)(2+3) + 2(3\times 4)(3+4) + 2(3\times 5)(3+5)\\
&\quad + 2(3\times 6)(3+6) + 2(3\times 7)(3+7) + 3(4\times 4)(4+4)\\
&\quad + 8(4\times 5)(4+5) + 5(5\times 5)(5+5) + (5\times 6)(5+6)\\
&\quad + 15(5\times 7)(5+7) + 3(5\times 8)(5+8) + (6\times 6)(6+6)\\
&\quad + 5(6\times 7)(6+7) + 2(6\times 8)(6+8) + 3(7\times 7)(7+7)\\
&\quad + 5(7\times 8)(7+8) + (8\times 8)(8+8)\\
&= 24264.
\end{aligned}
$$

(v) **Neighborhood forgotten index:**

$$
\begin{aligned}
F(\Upsilon) &= \sum_{st\in E(\Upsilon)} (\tau_\Upsilon(s)^2 + \tau_\Upsilon(t)^2)\\
&= 2(4+9) + 2(9+16) + 2(9+25) + 2(9+36) + 2(9+49)\\
&\quad + 3(16+16) + 8(16+25) + 5(25+25) + (25+36)\\
&\quad + 15(25+49) + 3(25+64) + (36+36) + 5(36+49)\\
&\quad + 2(36+64) + 3(49+49) + 5(49+64) + (64+64)\\
&= 4146.
\end{aligned}
$$

(vi) **Neighborhood general Randić index:**

$$\begin{aligned}
NR_\alpha(\Upsilon) &= \sum_{st\in E(\Upsilon)} (\tau_\Upsilon(s)\tau_\Upsilon(t))^\alpha \\
&= 2(2\times 3)^\alpha + 2(3\times 4)^\alpha + 2(3\times 5)^\alpha + 2(3\times 6)^\alpha + 2(3\times 7)^\alpha \\
&\quad + 3(4\times 4)^\alpha + 8(4\times 5)^\alpha + 5(5\times 5)^\alpha + (5\times 6)^\alpha + 15(5\times 7)^\alpha \\
&\quad + 3(5\times 8)^\alpha + (6\times 6)^\alpha + 5(6\times 7)^\alpha + 2(6\times 8)^\alpha + 3(7\times 7)^\alpha \\
&\quad + 5(7\times 8)^\alpha + (8\times 8)^\alpha \\
&= 2^{\alpha+1}\times 3^\alpha + 2^{2\alpha+1}\times 3^\alpha + 2\times 15^\alpha + 2^{\alpha+1}\times 3^{2\alpha} + 2\times 21^\alpha \\
&\quad + 3\times 2^{4\alpha} + 2^{2\alpha+3}\times 5^\alpha + 5^{2\alpha+1} + 30^\alpha + 3\times 5^{\alpha+1}\times 7^\alpha \\
&\quad + 3\times 2^{3\alpha}\times 5^\alpha + 6^{2\alpha} + 5\times 42^\alpha + 2^{4\alpha+1}\times 3^\alpha + 3\times 7^{2\alpha} \\
&\quad + 5\times 2^{3\alpha}\times 7^\alpha + 2^{6\alpha}.
\end{aligned}$$

(vii) **Neighborhood general inverse Randić index:**

$$\begin{aligned}
NRR_\alpha(\Upsilon) &= \sum_{st\in E(\Upsilon)} \frac{1}{(\tau_\Upsilon(s)\tau_\Upsilon(t))^\alpha} \\
&= \frac{2}{(2\times 3)^\alpha} + \frac{2}{(3\times 4)^\alpha} + \frac{2}{(3\times 5)^\alpha} + \frac{2}{(3\times 6)^\alpha} + \frac{2}{(3\times 7)^\alpha} \\
&\quad + \frac{3}{(4\times 4)^\alpha} + \frac{8}{(4\times 5)^\alpha} + \frac{5}{(5\times 5)^\alpha} + \frac{1}{(5\times 6)^\alpha} + \frac{15}{(5\times 7)^\alpha} \\
&\quad + \frac{3}{(5\times 8)^\alpha} + \frac{1}{(6\times 6)^\alpha} + \frac{5}{(6\times 7)^\alpha} + \frac{2}{(6\times 8)^\alpha} + \frac{3}{(7\times 7)^\alpha} \\
&\quad + \frac{5}{(7\times 8)^\alpha} + \frac{1}{(8\times 8)^\alpha} \\
&= \frac{1}{2^{\alpha-1}\times 3^\alpha} + \frac{2}{3^\alpha\times 4^\alpha} + \frac{2}{3^\alpha\times 5^\alpha} + \frac{2}{3^\alpha\times 6^\alpha} + \frac{2}{3^\alpha\times 7^\alpha} \\
&\quad + \frac{3}{4^{2\alpha}} + \frac{8}{4^\alpha\times 5^\alpha} + \frac{1}{5^{2\alpha-1}} + \frac{1}{5^\alpha\times 6^\alpha} + \frac{15}{5^\alpha\times 7^\alpha} + \frac{3}{5^\alpha\times 8^\alpha} \\
&\quad + \frac{1}{6^{2\alpha}} + \frac{5}{6^\alpha\times 7^\alpha} + \frac{2}{6^\alpha\times 8^\alpha} + \frac{3}{7^{2\alpha}} + \frac{5}{7^\alpha\times 8^\alpha} + \frac{1}{8^{2\alpha}}.
\end{aligned}$$

(viii) **Fifth NDe index:**

$$ND_5(\Upsilon) = \sum_{st\in E(\Upsilon)} \frac{\tau_\Upsilon(s)^2 + \tau_\Upsilon(t)^2}{\tau_\Upsilon(s)\tau_\Upsilon(t)}$$

$$
\begin{aligned}
&= 2\left\{\frac{4+9}{2\times 3}\right\} + 2\left\{\frac{9+16}{3\times 4}\right\} + 2\left\{\frac{9+25}{3\times 5}\right\} + 2\left\{\frac{9+36}{3\times 6}\right\} \\
&\quad + 2\left\{\frac{9+49}{3\times 7}\right\} + 3\left\{\frac{16+16}{4\times 4}\right\} + 8\left\{\frac{16+25}{4\times 5}\right\} + 5\left\{\frac{25+25}{5\times 5}\right\} \\
&\quad + \left\{\frac{25+36}{5\times 6}\right\} + 15\left\{\frac{25+49}{5\times 7}\right\} + 3\left\{\frac{25+64}{5\times 8}\right\} + \left\{\frac{36+36}{6\times 6}\right\} \\
&\quad + 5\left\{\frac{36+49}{6\times 7}\right\} + 2\left\{\frac{36+64}{6\times 8}\right\} + 3\left\{\frac{49+49}{7\times 7}\right\} + 5\left\{\frac{49+64}{7\times 8}\right\} \\
&\quad + \left\{\frac{64+64}{8\times 8}\right\} \\
&= \frac{54917}{420} \approx 130.7548.
\end{aligned}
$$

(ix) **Neighborhood harmonic index:**

$$
\begin{aligned}
NH(\Upsilon) &= \sum_{st\in E(\Upsilon)} \frac{2}{\tau_\Upsilon(s)+\tau_\Upsilon(t)} \\
&= 2\left\{\frac{2}{2+3}\right\} + 2\left\{\frac{2}{3+4}\right\} + 2\left\{\frac{2}{3+5}\right\} + 2\left\{\frac{2}{3+6}\right\} \\
&\quad + 2\left\{\frac{2}{3+7}\right\} + 3\left\{\frac{2}{4+4}\right\} + 8\left\{\frac{2}{4+5}\right\} + 5\left\{\frac{2}{5+5}\right\} \\
&\quad + \left\{\frac{2}{5+6}\right\} + 15\left\{\frac{2}{5+7}\right\} + 3\left\{\frac{2}{5+8}\right\} + \left\{\frac{2}{6+6}\right\} \\
&\quad + 5\left\{\frac{2}{6+7}\right\} + 2\left\{\frac{2}{6+8}\right\} + 3\left\{\frac{2}{7+7}\right\} + 5\left\{\frac{2}{7+8}\right\} \\
&\quad + \left\{\frac{2}{8+8}\right\} \\
&= \frac{4262647}{360360} \approx 11.8289.
\end{aligned}
$$

(x) **Neighborhood inverse sum index:**

$$
\begin{aligned}
NI(\Upsilon) &= \sum_{st\in E(\Upsilon)} \frac{\tau_\Upsilon(s)\tau_\Upsilon(t)}{\tau_\Upsilon(s)+\tau_\Upsilon(t)} \\
&= 2\left\{\frac{2\times 3}{2+3}\right\} + 2\left\{\frac{3\times 4}{3+4}\right\} + 2\left\{\frac{3\times 5}{3+5}\right\} + 2\left\{\frac{3\times 6}{3+6}\right\} + 2\left\{\frac{3\times 7}{3+7}\right\}
\end{aligned}
$$

$$+3\left\{\frac{4\times 4}{4+4}\right\}+8\left\{\frac{4\times 5}{4+5}\right\}+5\left\{\frac{5\times 5}{5+5}\right\}+\left\{\frac{5\times 6}{5+6}\right\}+15\left\{\frac{5\times 7}{5+7}\right\}$$
$$+3\left\{\frac{5\times 8}{5+8}\right\}+\left\{\frac{6\times 6}{6+6}\right\}+5\left\{\frac{6\times 7}{6+7}\right\}+2\left\{\frac{6\times 8}{6+8}\right\}+3\left\{\frac{7\times 7}{7+7}\right\}$$
$$+5\left\{\frac{7\times 8}{7+8}\right\}+\left\{\frac{8\times 8}{8+8}\right\}$$
$$=\frac{15219989}{90090}\approx 168.9420.$$

(xi) **Sanskruti index:**

$$S(\Upsilon)=\sum_{st\in E(\Upsilon)}\left\{\frac{\tau_\Upsilon(s)\tau_\Upsilon(t)}{\tau_\Upsilon(s)+\tau_\Upsilon(t)-2}\right\}^3$$
$$=2\left\{\frac{2\times 3}{2+3-2}\right\}^3+2\left\{\frac{3\times 4}{3+4-2}\right\}^3+2\left\{\frac{3\times 5}{3+5-2}\right\}^3$$
$$+2\left\{\frac{3\times 6}{3+6-2}\right\}^3+2\left\{\frac{3\times 7}{3+7-2}\right\}^3+3\left\{\frac{4\times 4}{4+4-2}\right\}^3$$
$$+8\left\{\frac{4\times 5}{4+5-2}\right\}^3+5\left\{\frac{5\times 5}{5+5-2}\right\}^3+\left\{\frac{5\times 6}{5+6-2}\right\}^3$$
$$+15\left\{\frac{5\times 7}{5+7-2}\right\}^3+3\left\{\frac{5\times 8}{5+8-2}\right\}^3+\left\{\frac{6\times 6}{6+6-2}\right\}^3$$
$$+5\left\{\frac{6\times 7}{6+7-2}\right\}^3+2\left\{\frac{6\times 8}{6+8-2}\right\}^3+3\left\{\frac{7\times 7}{7+7-2}\right\}^3$$
$$+5\left\{\frac{7\times 8}{7+8-2}\right\}^3+\left\{\frac{8\times 8}{8+8-2}\right\}^3$$
$$=\frac{4364153715096106937}{1733189185728000}\approx 2517.9904.$$

□

Further, the examination to determine the expression of NM-polynomial for the Zosurabalpin is performed in Theorem 9. Then, several corresponding neighborhood degree sum-based indices are enumerated by employing this NM-polynomial expression and formulas displayed in Table 1.

Theorem 9 *Let us denote the molecular graph of of Zosurabalpin as Υ. Then, the NM-polynomial expression of Zosurabalpin is given as*

$$NM(\Upsilon;x,y)=2x^2y^3+2x^3y^4+2x^3y^5+2x^3y^6+2x^3y^7+3x^4y^4+8x^4y^5$$

$$+ 5x^5y^5 + x^5y^6 + 15x^5y^7 + 3x^5y^8 + x^6y^6 + 5x^6y^7 + 2x^6y^8 + 3x^7y^7 + 5x^7y^8 + x^8y^8.$$

Proof: The neighborhood degree sum of each vertex of the hydrogen-suppressed 2D-molecular graph Υ of Zosurabalpin is depicted in Figure 5. The graph Υ contains 57 vertices and 62 edges, i.e. $|V(\Upsilon)| = 57$ and $|E(\Upsilon)| = 62$. Next, the possible feasible neighborhood degree sum of the vertices are $2, 3, 4, 5, 6, 7$ and 8. Furthermore, based on the neighborhood degrees sum of the end vertices of every edge, the division of the edge set $E(\Upsilon)$ into seventeen disjoint sets is represented as

$$E^*_{\{p,q\}} = \{e = st \in E(\Upsilon) : \tau(s) = p, \tau(t) = q\},$$

where $\{p, q\} = \{2, 3\}$, $\{3, 4\}$, $\{3, 5\}$, $\{3, 6\}$, $\{3, 7\}$, $\{4, 4\}$, $\{4, 5\}, \{5, 5\}$, $\{5, 6\}$, $\{5, 7\}$, $\{5, 8\}, \{6, 6\}$, $\{6, 7\},$, $\{6, 8\}$, $\{7, 7\}$ $\{7, 8\}$ and $\{8, 8\}$. Moreover, their cardinalities are given by $|E^*_{\{2,3\}}| = 2$, $|E^*_{\{3,4\}}| = 2$, $|E^*_{\{3,5\}}| = 2$, $|E^*_{\{3,6\}}| = 2$, $|E^*_{\{3,7\}}| = 2$, $|E^*_{\{4,4\}}| = 3$, $|E^*_{\{4,5\}}| = 8$, $|E^*_{\{5,5\}}| = 5$, $|E^*_{\{5,6\}}| = 1$, $|E^*_{\{5,7\}}| = 15$, $|E^*_{\{5,8\}}| = 3$, $|E^*_{\{6,6\}}| = 1$, $|E^*_{\{6,7\}}| = 5$, $|E^*_{\{6,8\}}| = 2$, $|E^*_{\{7,7\}}| = 3$, $|E^*_{\{7,8\}}| = 5$ and $|E^*_{\{8,8\}}| = 1$.

Therefore by Definition 2, the NM-polynomial of graph Υ is

$$\begin{aligned}
&NM(\Upsilon; x, y)\\
&= \sum_{p\leq q} \psi_{p,q}\, x^p y^q, \quad \text{where } p, q \in \{2, 3, 4, 5, 6, 7, 8\}\\
&= \sum_{2\leq 3} \psi_{2,3}\, x^2y^3 + \sum_{3\leq 4} \psi_{3,4}\, x^3y^4 + \sum_{3\leq 5} \psi_{3,5}\, x^3y^5 + \sum_{3\leq 6} \psi_{3,6}\, x^3y^6 + \sum_{3\leq 7} \psi_{3,7}\, x^3y^7\\
&\quad + \sum_{4\leq 4} \psi_{4,4}\, x^4y^4 + \sum_{4\leq 5} \psi_{4,5}\, x^4y^5 + \sum_{5\leq 5} \psi_{5,5}\, x^5y^5 + \sum_{5\leq 6} \psi_{5,6}\, x^5y^6 + \sum_{5\leq 7} \psi_{5,7}\, x^5y^7\\
&\quad + \sum_{5\leq 8} \psi_{5,8}\, x^5y^8 + \sum_{6\leq 6} \psi_{6,6}\, x^6y^6 + \sum_{6\leq 7} \psi_{6,7}\, x^6y^7 + \sum_{6\leq 8} \psi_{6,8}\, x^6y^8 + \sum_{7\leq 7} \psi_{7,7}\, x^7y^7\\
&\quad + \sum_{7\leq 8} \psi_{7,8}\, x^7y^8 + \sum_{8\leq 8} \psi_{8,8}\, x^8y^8\\
&= |E^*_{\{2,3\}}|\, x^2y^3 + |E^*_{\{3,4\}}|\, x^3y^4 + |E^*_{\{3,5\}}|\, x^3y^5 + |E^*_{\{3,6\}}|\, x^3y^6 + |E^*_{\{3,7\}}|\, x^3y^7\\
&\quad + |E^*_{\{4,4\}}|\, x^4y^4 + |E^*_{\{4,5\}}|\, x^4y^5 + |E^*_{\{5,5\}}|\, x^5y^5 + |E^*_{\{5,6\}}|\, x^5y^6 + |E^*_{\{5,7\}}|\, x^5y^7\\
&\quad + |E^*_{\{5,8\}}|\, x^5y^8 + |E^*_{\{6,6\}}|\, x^6y^6 + |E^*_{\{6,7\}}|\, x^6y^7 + |E^*_{\{6,8\}}|\, x^6y^8 + |E^*_{\{7,7\}}|\, x^7y^7\\
&\quad + |E^*_{\{7,8\}}|\, x^7y^8 + |E^*_{\{8,8\}}|\, x^8y^8\\
&= 2x^2y^3 + 2x^3y^4 + 2x^3y^5 + 2x^3y^6 + 2x^3y^7 + 3x^4y^4 + 8x^4y^5 + 5x^5y^5 + x^5y^6
\end{aligned}$$

$$+ 15x^5y^7 + 3x^5y^8 + x^6y^6 + 5x^6y^7 + 2x^6y^8 + 3x^7y^7 + 5x^7y^8 + x^8y^8.$$

□

Next, we make use of the graphic-polynomial approach to recover the various neighborhood degree sum-based topological indices using above-obtained NM-polynomial expression.

Proof: (*Alternative proof of Theorem* 8 using NM-polynomial approach). The NM-polynomial of Zosurabalpin (as evaluated in Theorem 9) is

$NM(\Upsilon; x, y) = 2x^2y^3 + 2x^3y^4 + 2x^3y^5 + 2x^3y^6 + 2x^3y^7 + 3x^4y^4 + 8x^4y^5 + 5x^5y^5 + x^5y^6 + 15x^5y^7 + 3x^5y^8 + x^6y^6 + 5x^6y^7 + 2x^6y^8 + 3x^7y^7 + 5x^7y^8 + x^8y^8$.

For simplicity of notations, we consider the function $g(x, y) = NM(\Upsilon; x, y)$. Now, we first compute the following essential operators over $g(x, y)$:

- $D_x(g(x, y)) = 4x^2y^3 + 6x^3y^4 + 6x^3y^5 + 6x^3y^6 + 6x^3y^7 + 12x^4y^4 + 32x^4y^5 + 25x^5y^5 + 5x^5y^6 + 75x^5y^7 + 15x^5y^8 + 6x^6y^6 + 30x^6y^7 + 12x^6y^8 + 21x^7y^7 + 35x^7y^8 + 8x^8y^8$,

- $D_y(g(x, y)) = 6x^2y^3 + 8x^3y^4 + 10x^3y^5 + 12x^3y^6 + 14x^3y^7 + 12x^4y^4 + 40x^4y^5 + 25x^5y^5 + 6x^5y^6 + 105x^5y^7 + 24x^5y^8 + 6x^6y^6 + 35x^6y^7 + 16x^6y^8 + 21x^7y^7 + 40x^7y^8 + 8x^8y^8$,

- $D_xD_y(g(x, y)) = 12x^2y^3 + 24x^3y^4 + 30x^3y^5 + 36x^3y^6 + 42x^3y^7 + 48x^4y^4 + 160x^4y^5 + 125x^5y^5 + 30x^5y^6 + 525x^5y^7 + 120x^5y^8 + 36x^6y^6 + 210x^6y^7 + 96x^6y^8 + 147x^7y^7 + 280x^7y^8 + 64x^8y^8$,

- $(D_x + D_y)(g(x, y)) = 10x^2y^3 + 14x^3y^4 + 16x^3y^5 + 18x^3y^6 + 20x^3y^7 + 24x^4y^4 + 72x^4y^5 + 50x^5y^5 + 11x^5y^6 + 180x^5y^7 + 39x^5y^8 + 12x^6y^6 + 65x^6y^7 + 28x^6y^8 + 42x^7y^7 + 75x^7y^8 + 16x^8y^8$,

- $(D_xD_y)(D_x + D_y)(g(x, y)) = 60x^2y^3 + 168x^3y^4 + 240x^3y^5 + 324x^3y^6 + 420x^3y^7 + 384x^4y^4 + 1440x^4y^5 + 1250x^5y^5 + 330x^5y^6 + 6300x^5y^7 + 1560x^5y^8 + 432x^6y^6 + 2730x^6y^7 + 1344x^6y^8 + 2058x^7y^7 + 4200x^7y^8 + 1024x^8y^8$,

- $S_x(g(x, y)) = x^2y^3 + \frac{2}{3}x^3y^4 + \frac{2}{3}x^3y^5 + \frac{2}{3}x^3y^6 + \frac{2}{3}x^3y^7 + \frac{3}{4}x^4y^4 + 2x^4y^5 + x^5y^5 + \frac{1}{5}x^5y^6 + 3x^5y^7 + \frac{3}{5}x^5y^8 + \frac{1}{6}x^6y^6 + \frac{5}{6}x^6y^7 + \frac{1}{3}x^6y^8 + \frac{3}{7}x^7y^7 + \frac{5}{7}x^7y^8 + \frac{1}{8}x^8y^8$,

- $D_yS_x(g(x, y)) = 3x^2y^3 + \frac{8}{3}x^3y^4 + \frac{10}{3}x^3y^5 + 4x^3y^6 + \frac{14}{3}x^3y^7 + 3x^4y^4 + 10x^4y^5 + 5x^5y^5 + \frac{6}{5}x^5y^6 + 21x^5y^7 + \frac{24}{5}x^5y^8 + x^6y^6 + \frac{35}{6}x^6y^7 + \frac{8}{3}x^6y^8 + 3x^7y^7 + \frac{40}{7}x^7y^8 + x^8y^8$,

- $S_y(g(x,y)) = \frac{2}{3}x^2y^3+\frac{1}{2}x^3y^4+\frac{2}{5}x^3y^5+\frac{1}{3}x^3y^6+\frac{2}{7}x^3y^7+\frac{3}{4}x^4y^4+\frac{8}{5}x^4y^5+x^5y^5+\frac{1}{6}x^5y^6+\frac{15}{7}x^5y^7+\frac{3}{8}x^5y^8+\frac{1}{6}x^6y^6+\frac{5}{7}x^6y^7+\frac{1}{4}x^6y^8+\frac{3}{7}x^7y^7+\frac{5}{8}x^7y^8+\frac{1}{8}x^8y^8$,
- $D_xS_y(g(x,y)) = \frac{4}{3}x^2y^3+\frac{3}{2}x^3y^4+\frac{6}{5}x^3y^5+x^3y^6+\frac{6}{7}x^3y^7+3x^4y^4+\frac{32}{5}x^4y^5+5x^5y^5+\frac{5}{6}x^5y^6+\frac{75}{7}x^5y^7+\frac{15}{8}x^5y^8+x^6y^6+\frac{30}{7}x^6y^7+\frac{3}{2}x^6y^8+3x^7y^7+\frac{35}{8}x^7y^8+x^8y^8$,
- $S_xS_y(g(x,y)) = \frac{1}{3}x^2y^3+\frac{1}{6}x^3y^4+\frac{2}{15}x^3y^5+\frac{1}{9}x^3y^6+\frac{2}{21}x^3y^7+\frac{3}{16}x^4y^4+\frac{2}{5}x^4y^5+\frac{1}{5}x^5y^5+\frac{1}{30}x^5y^6+\frac{3}{7}x^5y^7+\frac{3}{40}x^5y^8+\frac{1}{36}x^6y^6+\frac{5}{42}x^6y^7+\frac{1}{24}x^6y^8+\frac{3}{49}x^7y^7+\frac{5}{56}x^7y^8+\frac{1}{64}x^8y^8$,
- $D_x^\alpha D_y^\alpha(g(x,y)) = 2^{\alpha+1}\times3^\alpha x^2y^3+2^{2\alpha+1}\times3^\alpha x^3y^4+2\times15^\alpha x^3y^5+2^{\alpha+1}\times3^{2\alpha}x^3y^6+2\times21^\alpha x^3y^7+3\times2^{4\alpha}x^4y^4+2^{2\alpha+3}\times5^\alpha x^4y^5+5^{2\alpha+1}x^5y^5+30^\alpha x^5y^6+3\times5^{\alpha+1}\times7^\alpha x^5y^7+3\times2^{3\alpha}\times5^\alpha x^5y^8+6^{2\alpha}x^6y^6+5\times42^\alpha x^6y^7+2^{4\alpha+1}\times3^\alpha x^6y^8+3\times7^{2\alpha}x^7y^7+5\times2^{3\alpha}\times7^\alpha x^7y^8+2^{6\alpha}x^8y^8$,
- $S_x^\alpha S_y^\alpha(g(x,y)) = \frac{1}{2^{\alpha-1}\times3^\alpha}x^2y^3+\frac{2}{3^\alpha\times4^\alpha}x^3y^4+\frac{2}{3^\alpha\times5^\alpha}x^3y^5+\frac{2}{3^\alpha\times6^\alpha}x^3y^6+\frac{2}{3^\alpha\times7^\alpha}x^3y^7+\frac{3}{4^{2\alpha}}x^4y^4+\frac{8}{4^\alpha\times5^\alpha}x^4y^5+\frac{1}{5^{2\alpha-1}}x^5y^5+\frac{1}{5^\alpha\times6^\alpha}x^5y^6+\frac{15}{5^\alpha\times7^\alpha}x^5y^7+\frac{3}{5^\alpha\times8^\alpha}x^5y^8+\frac{1}{6^{2\alpha}}x^6y^6+\frac{5}{6^\alpha\times7^\alpha}x^6y^7+\frac{2}{6^\alpha\times8^\alpha}x^6y^8+\frac{3}{7^{2\alpha}}x^7y^7+\frac{5}{7^\alpha\times8^\alpha}x^7y^8+\frac{1}{8^{2\alpha}}x^8y^8$,
- $(D_xS_y+D_yS_x)(g(x,y)) = \frac{13}{3}x^2y^3+\frac{25}{6}x^3y^4+\frac{68}{15}x^3y^5+5x^3y^6+\frac{116}{21}x^3y^7+6x^4y^4+\frac{82}{5}x^4y^5+10x^5y^5+\frac{61}{30}x^5y^6+\frac{222}{7}x^5y^7+\frac{267}{40}x^5y^8+2x^6y^6+\frac{425}{42}x^6y^7+\frac{25}{6}x^6y^8+6x^7y^7+\frac{565}{56}x^7y^8+2x^8y^8$,
- $S_xJ(g(x,y)) = \frac{2}{5}x^5+\frac{2}{7}x^7+\frac{5}{8}x^8+\frac{10}{9}x^9+\frac{7}{10}x^{10}+\frac{1}{11}x^{11}+\frac{4}{3}x^{12}+\frac{8}{13}x^{13}+\frac{5}{14}x^{14}+\frac{1}{3}x^{15}+\frac{1}{16}x^{16}$,
- $S_xJD_xD_y(g(x,y)) = \frac{12}{5}x^5+\frac{24}{7}x^7+\frac{39}{4}x^8+\frac{196}{9}x^9+\frac{167}{10}x^{10}+\frac{30}{11}x^{11}+\frac{187}{4}x^{12}+\frac{330}{13}x^{13}+\frac{243}{14}x^{14}+\frac{56}{3}x^{15}+4x^{16}$,
- $S_x^3Q_{-2}JD_x^3D_y^3(g(x,y)) = \frac{432}{27}x^3+\frac{3456}{125}x^5+\frac{19038}{216}x^6+\frac{75664}{343}x^7+\frac{96647}{512}x^8+\frac{1000}{27}x^9+\frac{689781}{1000}x^{10}+\frac{562440}{1331}x^{11}+\frac{574131}{1728}x^{12}+\frac{878080}{2197}x^{13}+\frac{32768}{343}x^{14}$.

Thus, using the derivation formulas cataloged in 1, the neighborhood degree sum-based topological indices of Zosurabalpin are as follows:

(i) **Neighborhood First Zagreb Index:**

$$NM_1(\Upsilon) = (D_x+D_y)(g(x,y))|_{x=y=1} = 692.$$

(*ii*) **Neighborhood Second Zagreb Index:**

$$NM_2(\Upsilon) = D_x D_y(g(x,y))|_{x=y=1} = 1985.$$

(*iii*) **Neighborhood Modified Second Zagreb Index:**

$${}^{nm}M_2(\Upsilon) = S_x S_y(g(x,y))|_{x=y=1} = \frac{355441}{141120} \approx 2.5187..$$

(*iv*) **Third NDe Index:**

$$ND_3(\Upsilon) = D_x D_y(D_x + D_y)(g(x,y))|_{x=y=1} = 24264.$$

(*v*) **Neighborhood Forgotten Index:**

$$NF(\Upsilon) = (D_x^2 + D_y^2)(g(x,y))|_{x=y=1} = 4146.$$

(*vi*) **Neighborhood General Randić Index:**

$$\begin{aligned} NR_\alpha(\Upsilon) &= D_x^\alpha D_y^\alpha(g(x,y))|_{x=y=1} \\ &= 2^{\alpha+1}\times 3^\alpha + 2^{2\alpha+1}\times 3^\alpha + 2\times 15^\alpha + 2^{\alpha+1}\times 3^{2\alpha} + 2\times 21^\alpha \\ &\quad + 3\times 2^{4\alpha} + 2^{2\alpha+3}\times 5^\alpha + 5^{2\alpha+1} + 30^\alpha + 3\times 5^{\alpha+1}\times 7^\alpha \\ &\quad + 3\times 2^{3\alpha}\times 5^\alpha + 6^{2\alpha} + 5\times 42^\alpha + 2^{4\alpha+1}\times 3^\alpha + 3\times 7^{2\alpha} \\ &\quad + 5\times 2^{3\alpha}\times 7^\alpha + 2^{6\alpha}. \end{aligned}$$

(*vii*) **Neighborhood General Inverse Randić Index:**

$$\begin{aligned} NRR_\alpha(\Upsilon) &= S_x^\alpha S_y^\alpha(g(x,y))|_{x=y=1} \\ &= \frac{1}{2^{\alpha-1}\times 3^\alpha} + \frac{2}{3^\alpha\times 4^\alpha} + \frac{2}{3^\alpha\times 5^\alpha} + \frac{2}{3^\alpha\times 6^\alpha} + \frac{2}{3^\alpha\times 7^\alpha} \\ &\quad + \frac{3}{4^{2\alpha}} + \frac{8}{4^\alpha\times 5^\alpha} + \frac{1}{5^{2\alpha-1}} + \frac{1}{5^\alpha\times 6^\alpha} + \frac{15}{5^\alpha\times 7^\alpha} + \frac{3}{5^\alpha\times 8^\alpha} \\ &\quad + \frac{1}{6^{2\alpha}} + \frac{5}{6^\alpha\times 7^\alpha} + \frac{2}{6^\alpha\times 8^\alpha} + \frac{3}{7^{2\alpha}} + \frac{5}{7^\alpha\times 8^\alpha} + \frac{1}{8^{2\alpha}}. \end{aligned}$$

(*viii*) **Fifth NDe Index:**

$$ND_5(\Upsilon) = (D_x S_y + D_y S_x)(g(x,y))|_{x=y=1} = \frac{54917}{420} \approx 130.7548.$$

(ix) **Neighborhood Harmonic Index:**

$$NH(\Upsilon) = 2S_xJ(g(x,y))|_{x=1} = \frac{4262647}{360360} \approx 11.8289.$$

(x) **Neighborhood Inverse Sum (Indeg) Index:**

$$NI(\Upsilon) = S_xJD_xD_y(g(x,y))|_{x=1} = \frac{15219989}{90090} \approx 168.9420.$$

(xi) **Sanskruti Index:**

$$S(\Upsilon) = S_x^3Q_{-2}JD_x^3D_y^3(g(x,y))|_{x=1} = \frac{4364153715096106937}{1733189185728000} \approx 2517.9904.$$

□

Corollary 10 *Theorem 8 demonstrate that the expression of the neighborhood general Randić index of a graph Υ is represented as* $NR_\alpha(\Upsilon) = 2^{\alpha+1} \times 3^\alpha + 2^{2\alpha+1} \times 3^\alpha + 2 \times 15^\alpha + 2^{\alpha+1} \times 3^{2\alpha} + 2 \times 21^\alpha + 3 \times 2^{4\alpha} + 2^{2\alpha+3} \times 5^\alpha + 5^{2\alpha+1} + 30^\alpha + 3 \times 5^{\alpha+1} \times 7^\alpha + 3 \times 2^{3\alpha} \times 5^\alpha + 6^{2\alpha} + 5 \times 42^\alpha + 2^{4\alpha+1} \times 3^\alpha + 3 \times 7^{2\alpha} + 5 \times 2^{3\alpha} \times 7^\alpha + 2^{6\alpha}$. *For $\alpha = -1/2$, It is known as the neighborhood Randić index of Υ and its value is* $NR_{-1/2}(\Upsilon) = 11.9979$.

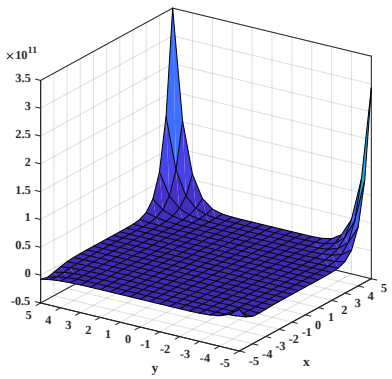
Corollary 11 *On the contrary, Theorem 8 describes that the expression of the neighborhood general inverse Randić index of a graph Υ is denoted and calculated by* $NRR_\alpha(\Upsilon) = \frac{1}{2^{\alpha-1} \times 3^\alpha} + \frac{2}{3^\alpha \times 4^\alpha} + \frac{2}{3^\alpha \times 5^\alpha} + \frac{2}{3^\alpha \times 6^\alpha} + \frac{2}{3^\alpha \times 7^\alpha} + \frac{3}{4^{2\alpha}} + \frac{8}{4^\alpha \times 5^\alpha} + \frac{1}{5^{2\alpha-1}} + \frac{1}{5^\alpha \times 6^\alpha} + \frac{15}{5^\alpha \times 7^\alpha} + \frac{3}{5^\alpha \times 8^\alpha} + \frac{1}{6^{2\alpha}} + \frac{5}{6^\alpha \times 7^\alpha} + \frac{2}{6^\alpha \times 8^\alpha} + \frac{3}{7^{2\alpha}} + \frac{5}{7^\alpha \times 8^\alpha} + \frac{1}{8^{2\alpha}}$, *$NRR_\alpha(\Upsilon)$ is known as the first NDe index of Υ and its value is given by* $ND_1(\Upsilon) = 341.8649$.

Remark 12 *The numerical values of the various neighborhood degree sum-based topological indices that were taken into consideration from the NM-polynomial technique match the values that were produced by applying the usual mathematical definitions.*

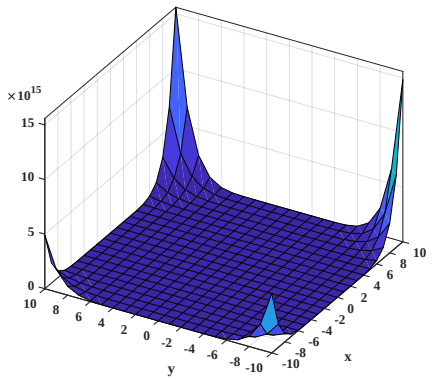
Furthermore, the 3D-surface representation of the NM-polynomial of Zosurabalpin is presented in Figure 6 for different ranges of x and y using MATLAB R2019a software. For example, we geometrically depict the polynomial in different ranges as shown in Figure 6(a) for $-5 \leq x, y \leq 5$, Figure 6(b) for $-10 \leq x, y \leq 10$ and Figure 6(c) for $-20 \leq x, y \leq 20$. Observed that,

these surfaces seem to behave similarly, but in reality, their gradients vary depending on the location whose coordinates are based on the parameters x and y. The values of the neighborhood degree sum-based topological indices is demonstrated in Figure 7 and are arranged in ascending order using MS Excel. Figure 7 signifies that the third NDe index (ND_3) observe the highest numerical value $24,264$ while the neighborhood modified second Zagreb (${}^{nm}M_2$) have the lowest value 2.5187. The neighborhood degree sum-based topological indices preserve the following inequality relationship:

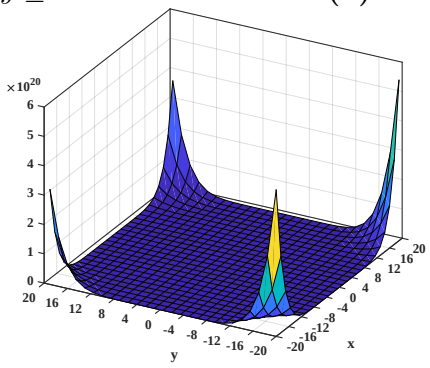
$${}^{nm}M_2 < NH < NR_{-1/2} < ND_5 < NI < ND_1 < NM_1 < NM_2 < S < NF < ND_3.$$



(a) For $-5 \leq x, y \leq 5$



(b) For $-10 \leq x, y \leq 10$



(c) For $-20 \leq x, y \leq 20$

Figure 6: Surface depiction of NM-polynomial of Zosurabalpin for different regions of x and y.

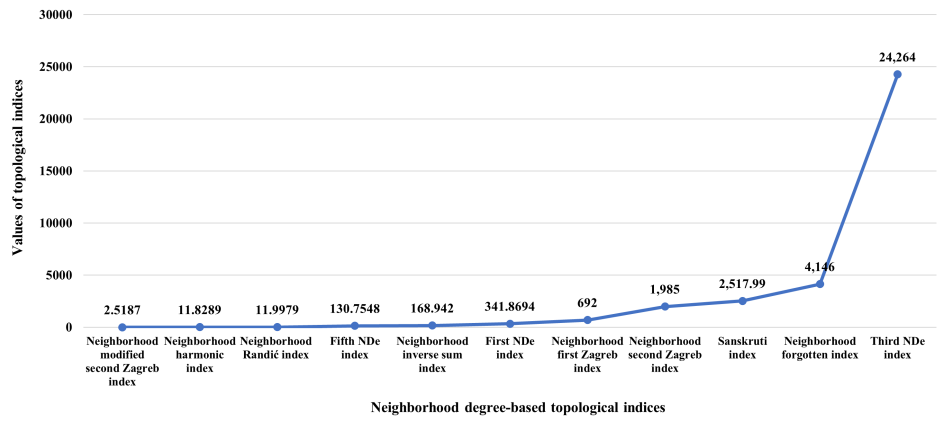


Figure 7: Graphical plot of the numerical values of neighborhood degree sum-based topological indices of Zosurabalpin in increasing order.

4 A Comparative Analysis

In this section, we present a comparative study between degree-based and associated neighborhood degree sum-based topological indices of Zosurabalpin. Keeping in mind the diversity of the value range of the topological indices, we have partitioned the topological indices in two parts. Accordingly, the comparison of numerical values of both classes of topological indices are shown in Tables 2 and 3, and their associated Figures 8 and 9 are plotted using 2D-line plot in MS Excel. We extract from Figure 8 that, apart from the *ISI*

Table 2: Comparative values of the degree-based topological indices ($^{m}M_2$, H, $R_{-1/2}$, *ISI*, *SDD* and $RR_{-1/2}$) and their associated neighborhood versions of topological indices of Zosurabalpin.

Sl. No.	**Degree-based**		**Neighborhood degree sum-based**	
	DBTI	**Numerical value**	**NDSBTI**	**Numerical value**
1.	$^{m}M_2$	12.8333	$^{nm}M_2$	2.5187
2.	H	26.9333	NH	11.8289
3.	$R_{-1/2}$	27.6763	$NR_{-1/2}$	11.9979
4.	*ISI*	70.6333	*NI*	168.9420
5.	*SDD*	137.0000	ND_5	130.7548
6.	$RR_{-1/2}$	144.0085	ND_1	341.8694

and $RR_{-1/2}$ indices, the degree-based topological indices have higher values in comparison to their associated neighborhood versions. Whereas Figure 9

depicts that the neighborhood degree sum-based topological indices have a higher value in comparison to their associated degree-based topological indices.

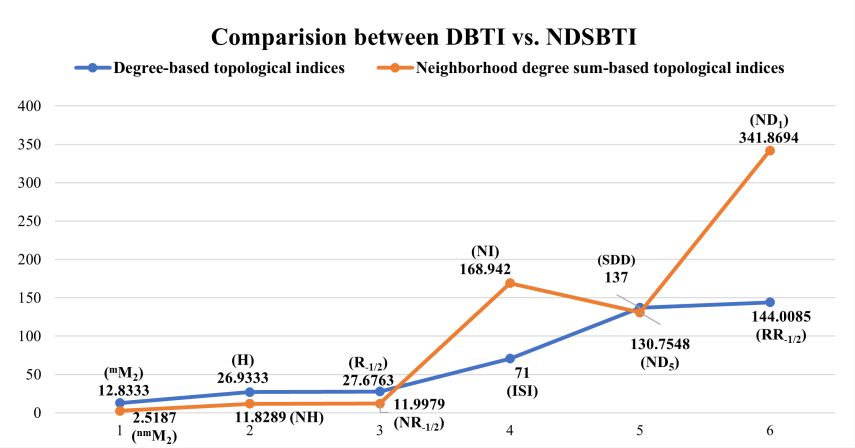


Figure 8: Comparison between degree-based (${}^{m}M_2$, H, $R_{-1/2}$, ISI, SDD and $RR_{-1/2}$) and associated neighborhood degree sum-based topological indices.

Table 3: Comparative values of the degree-based topological indices (M_1, M_2, AZI, F and $ReZG_3$) and their associated neighborhood versions of topological indices of Zosurabalpin.

Sl. No.	Degree-based		Neighborhood degree sum-based	
	DBTI	Numerical value	NDSBTI	Numerical value
1.	M_1	294.0000	NM_1	692.0000
2.	M_2	346.0000	NM_2	1,985.0000
3.	AZI	508.9375	S	2517.9900
4.	F	742.0000	NF	4,146.0000
5.	$ReZG_3$	1,740.0000	ND_3	24,264.0000

5 Conclusion

In this research article, the topological characterization of Zosurabalpin is presented using the degree-based and neighborhood degree sum-based topological indices. The degree-based and neighborhood degree sum-based topological indices of the antibiotic drug Zosurabalpin were computed using

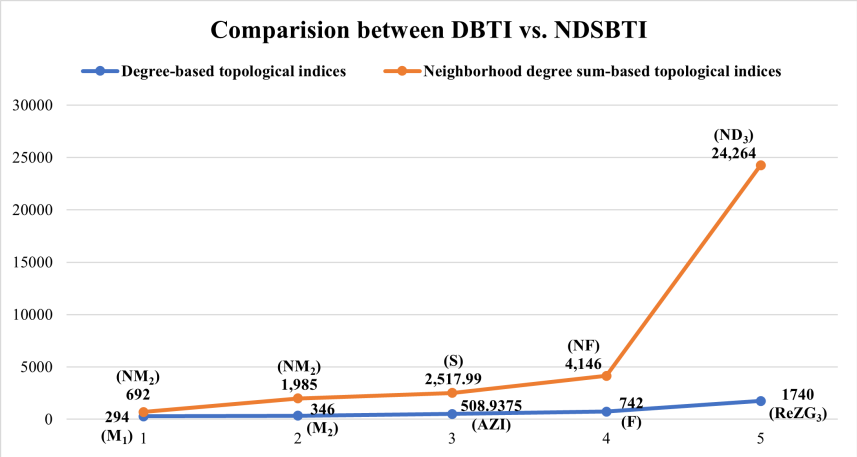


Figure 9: Comparison between degree-based (M_1, M_2, AZI, F and $ReZG_3$) and associated neighborhood degree sum-based topological indices.

M-polynomial and NM-polynomial, respectively. From a verification point of view, the computation of both classes of indices is also evaluated with the help of the mathematical definition of the respective topological indices. Eventually, we obtained identical results from both computational methods. The geometrical behaviour of M-polynomial and NM-polynomial were depicted in the different ranges of x and y. Numerical values of both types of indices were plotted in increasing order using MS Excel. Our performed comparative analysis showed that most of neighborhood degree sum-based topological indices obtained higher values in comparison to the associated degree-based topological indices, apart from ${}^{nm}M_2$, NH, $NR_{-1/2}$ and ND_5 indices. The obtained values of topological indices may be beneficial to the researchers working in the area of drug design to predict the physicochemical properties of Zosurabalpin through Quantitative Structure-Property Relationship analysis.

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Author Contributions

All the authors contributed equally to this work.

Data Availability Statement

The data used to support the findings of this study are included within the article.

Disclosure Statement & Competing Interests

No disclosure statement and potential conflict of interest was reported by the authors.

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